

Phenol, 4-chloro-2-methoxy-
16766-30-6 | DTXSID0074974

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: 32.0 °C

Global applicability domain: Inside

Local applicability domain index: 6.06e-01

Confidence level: 5.14e-01

Nearest Neighbors from the Training Set

Image not found

Phenol, 4-chloro-2-methoxy-

Measured: 16.5

Predicted: 32.0

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Benzoic acid, 5-chloro-2-hydroxy-, methyl ester

Measured: 50.0

Predicted: 45.1

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5-Chlorosalicylaldehyde

Measured: 100

Predicted: 72.9

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Salicyloyl chloride

Measured: 19.0

Predicted: 57.5

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3,5-Dichlorobenzyl alcohol

Measured: 80.5

Predicted: 68.8